Russian Journal of General Chemistry 2008 vol.78 N2, pages 277-280

Theoretical conformational analysis of substituted nitroethenes in solution

Chachkov D., Gazizova A., Vereshchagina Y., Ishmaeva E., Berestovitskaya V.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

Theoretical conformational analysis of 1-nitro- and 1-bromo-1-nitro-2- (trichloromethyl)ethenes dissolved in methylene chloride and benzene was carried out by the B3LYP/6-31G*method. The calculated structures of these compounds were found to nicely fit experiment: Both in the gas phase and in solution, 1-nitro-(2-trichloromethyl)ethene is an E isomer, while its bromine-containing analog is a Z isomer. © 2008 MAIK Nauka.

http://dx.doi.org/10.1007/s11176-008-2016-8